

Nontarget Screening of Organic Pollutants in Swedish Waters

May Britt Rian, Bénilde Bonnefille & Jonathan Martin

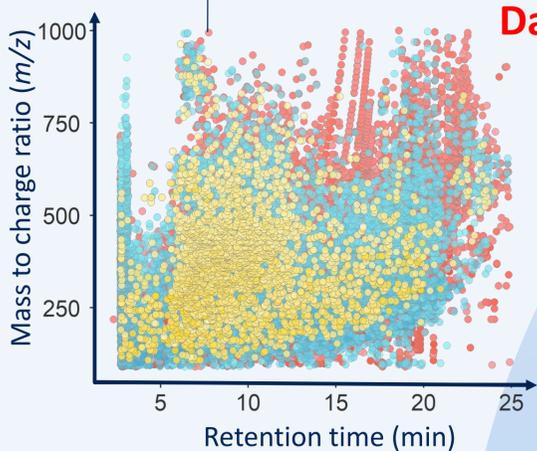
Department of Environmental Science, Exposure and Effects Unit (ACESx), Science for Life Laboratory, Stockholm University



Nontarget Screening

Monitoring of organic pollutants has traditionally been focusing on small groups of well-defined chemicals. Nontargeted High Resolution Mass Spectrometry (HRMS)-based screening can overcome this limitation, collecting signals for all detectable compounds in the samples.

One feature: accurate mass, fragment masses, retention time, intensity



Data acquisition and pre-processing

Majority of water pollution is unknown

Simple but comprehensive screening workflow

Early warning

Accelerate the discovery of novel and unknown contaminants

Publicly available archive with chemical information

Spectral library match

In silico fragmentation

NO MATCH

Molecular Networking

- Ground waters
- Waste waters
- Surface Waters
- Drinking waters

Acknowledge for organizing sampling:



WP3: Hazard and risk screening – early warning and proactivity

